Parastatistics of charged bosons partly localised by impurities

A.S. Alexandrov, R.T. Giles

Department of Physics, Loughborough University, Loughborough, LE11 3TU, U.K.

(February 1, 2008)

Coulomb repulsion is taken into account to derive the thermodynamics of charged bosons in a random external potential. A simple analytical form of the partition function is proposed for the case of non-overlapping localised states (i.e. a small amount of disorder). The density of localised bosons and the specific heat show a peculiar non-uniform temperature dependence below the Bose-Einstein condensation temperature. The superfluid - Bose-glass phase diagram is discussed. A new phase is predicted which is a Bose-glass at $T = 0$ but a superfluid at finite T.

74.20.-z,74.65.+n,74.60.Mj

I. INTRODUCTION

The charged Bose-gas (CBG), being an important reference system of quantum statistics, has become of particular physical interest in the field of high temperature superconductivity[1]. A long time ago Schafroth[2] demonstrated that an ideal gas of charged bosons exhibits the Meissner-Ochsenfeld effect below the ideal Bose-gas condensation temperature. Later, the one-particle excitation spectrum at $T = 0$ was calculated by Foldy[3] who worked at zero temperature using the Bogoliubov[4] approach. The Bogoliubov method leads to the result that the elementary excitations of the system have, for small momenta, energies characteristic of plasma oscillations which pass over smoothly for large momenta to the energies characteristic of single particle excitations. Further investigations have been carried out at or near T_c, the transition temperature for the gas; these have been concerned with the critical exponents[5] and the change in the transition temperature from that of the ideal gas[6,5]. The RPA dielectric response function and screening in a CBG have been studied in the high-density limit[7,8]. The theory of the CBG beyond the lowest order Bogoliubov approximation was discussed by Lee and Feenberg[9] and by Brueckner[10], both of whom obtained the next order correction to the ground state energy. Woo and Ma[11] calculated numerically the correction to the Bogoliubov excitation spectrum. Alexandrov[12] found the critical magnetic field $H_{c2}(T)$ at which the CBG is condensed; the predicted temperature dependence of H_{c2} was observed both in low-T_c and high-T_c cuprates, in which the coherence volume estimated from the heat capacity measurements is comparable with or even less than the unit cell volume.

The doped Mott insulators are intrinsically disordered.

Hence, the localisation of carriers in a random potential plays a crucial role in their low-temperature thermodynamics and transport properties. As an example, if a fraction of bipolarons is localised by disorder and the Coulomb repulsion in localised states is sufficiently strong, then the number of delocalised bosons is proportional to T while the boson-boson inelastic scattering rate is proportional to T^2; this can explain both the linear temperature dependence of the in-plane resistivity and the Hall density observed in the cuprates[1]. The picture of interacting bosons with a short-range interaction filling up all localised single-particle states in a random potential and Bose-condensing into the first extended state is known in the literature[13–15]. To calculate the density of localised bosons one has to take into account the repulsion between them. One cannot ignore the fact that the localisation length ξ generally varies with energy and diverges at the mobility edge. One would expect that the number of *hard core* bosons in a localised state near the mobility edge diverges in a similar way to the localisation length. Therefore only a repulsive interaction can stop all particles condensing into the lowest localised state. Thus, as stressed by Fisher *et al*[15], there is no sensible non-interacting starting point in the Bose gas about which to perturb (in contrast to the Fermi gas).

The scaling analysis of neutral bosons in random potentials by Fisher *et al*[15] describes the Bose-glass - superfluid phase transition at zero temperature with the increasing density and (or) the hopping strength. However the analysis is limited to the critical region near the transition and predicts[16] the universal resistance R^* at the Mott insulator to superconductor transition (in two dimensions) while data[17] on amorphous films suggest a wide range of R^*. Simple analytically solvable models of interacting bosons in a random potential might therefore be helpful. Lee and Gunn[18] proposed a picture of neutral bosons in which the "true" extended Bose condensate coexists with bosons in localised states. In this paper we develop a similar model for charged bosons interacting via Coulomb forces.

The number of *charged* bosons in a single potential well is determined by the competition between the long-range Coulomb potential energy $\simeq 4e^2/\epsilon_0\xi$ and the binding energy $E_c - E$, where ϵ_0 is the background dielectric constant and E_c is the mobility edge. If the Coulomb interaction is strong and the localisation length ξ diverges as $\xi \propto (E_c - E)^{-\nu}$ with $\nu < 1$, then each potential well cannot contain more than one boson[1]. Within this approximation the localised bosons obey Fermi-Dirac statistics because Coulomb repulsion has the same effect as

1

the Pauli exclusion principle. In the extreme case of the hydrogen atom the average electron-nucleus distance is inversely proportional to the binding energy, i.e. $\nu = 1$. The hydrogen negative ion exists but with rather low electron affinity so the doubly charged negative ion H^{2-} exists only as a resonant state. However, in general, the exponent ν can be larger then unity and the Coulomb repulsion is not infinite, so the statistics of localised charged bosons is neither Bose nor Fermi.

In this paper we study the parastatistics of partly localised charged bosons in the superfluid phase. In this phase the chemical potential μ is exactly at the mobility edge, $\mu = E_c$. We assume that the density of bosons n is not very high or the dimensionality is reduced so the localised states are not completely screened out (as in the case of the Mott transition in semiconductors). For a $3D$ system that means that the dimensionless strength of the Coulomb repulsion should be about unity or larger, $r_s = 4me^2/\epsilon_0(4\pi n/3)^{1/3} \geq 1$ where m is the boson mass and we take $\hbar = 1$. At the same time the density should not be extremely low if delocalised bosons are in a superfluid phase. A rather large magnitude of $r_s >> 1$ is necessary for the Wigner crystallisation of charged carriers. Therefore, the above condition takes place practically in the whole relevant region of the carrier density. Moreover in reduced dimensions, relevant for cuprates, the localised states cannot be screened out even if $r_s \leq 1$, and for $r_s > 1$ the localisation length ξ is essentially unaffected by delocalised bosons or the Bogoliubov collective mode. Hence our picture suggests that some particles remain in localised states while others are in the "true" extended Bose condensate; for neutral bosons this picture has been justified by Lee and Gunn[18].

II. PARTITION FUNCTION OF LOCALISED CHARGED BOSONS

The Hamiltonian of charged bosons on an oppositely charged background (to ensure charge neutrality) in an external random field with the potential $U(\mathbf{r})$ is given by

$$H = \int d\mathbf{r}\psi^\dagger(\mathbf{r})\left[-\frac{\nabla^2}{2m} - \mu + U(\mathbf{r})\right]\psi(\mathbf{r})$$
$$+ \frac{1}{2}\int d\mathbf{r}\int d\mathbf{r}'V(\mathbf{r}-\mathbf{r}')\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\psi^\dagger(\mathbf{r}')\psi(\mathbf{r}'). \quad (1)$$

The Fourier component of the Coulomb potential for bosonic charge $2e$ is $V(\mathbf{k}) = 16\pi e^2/\epsilon_0 k^2$ in a $3D$ system, and $V(\mathbf{k}) = 8\pi e^2/\epsilon_0 k$ in a $2D$ system with a three dimensional interaction. For a low amount of disorder a single particle spectrum consists of localised discrete levels below the bottom of the conduction band E_c. At some finite temperature, T_c, bosons are condensed at $E = E_c$ so that $\mu = E_c$. If the Coulomb repulsion is strong one can expect that each localised state below E_c is occupied by one or a few bosons. The excitation spectrum of the delocalised charged superfluid has a gap of the order of

the plasma frequency[3]. Therefore the low-temperature thermodynamics is controlled by the excitation of the shallow localised states while the Bogoliubov collective modes can be ignored. In $3D$ their contribution is exponentially small while in $2D$ their energy scales as T^5 and the specific heat as T^4. Even in the case of a short range repulsion the sound modes yield an energy proportional to T^{d+1} and hence a specific heat which behaves like $C \propto T^d$ (where d stands for the dimensionality)[15]. Therefore the contribution to thermodynamics from the delocalised bosons appears to be negligible at low temperatures compared with that from bosons localised in shallow potential wells for $d \geq 2$. So in the following we calculate the partition function and specific heat of localised bosons only.

When two or more charged bosons are in a single localised state of energy E there may be significant Coulomb energy and we try to take this into account as follows. The localisation length ξ is assumed to depend on E via

$$\xi \sim \frac{1}{(-E)^\nu}, \quad (2)$$

where $\nu > 0$. The Coulomb energy of p charged bosons confined within a radius ξ can be expected to be of order

$$\frac{p(p-1)e^2}{\epsilon_0\xi}. \quad (3)$$

Thus the total energy w of p bosons in a localised state of energy E is taken to be

$$w = pE + p(p-1)\kappa(-E)^\nu \quad (4)$$

where $\kappa > 0$. Hence, as mentioned above, we see that the behaviour of charged bosons in localised states can be thought of as intermediate between Bose-Einstein statistics and Fermi-Dirac statistics. When $\kappa = 0$ we have an equally spaced set of levels, i.e. Bose-Einstein behaviour, whereas when $\kappa = \infty$ we have Fermi-Dirac behaviour since the only levels with finite energy are $p = 0$ and $p = 1$, and thus an exclusion principle is enforced. When $0 < \kappa < \infty$ we have the intermediate 'parastatistics' that the level spacing $\delta w \to \infty$ as $p \to \infty$. This behaviour is closely analagous to that observed in the Coulomb blockade model which applies to quantum dots[19].

We are primarily interested in the properties of the superconducting phase, namely the phase in which a true (extended) Bose condensate is present. The only state in which the true condensate can form is the lowest energy delocalised state E_c. Hence, when there is a Bose condensate, the chemical potential μ must be equal to zero if we choose $E_c = 0$.

We take the total energy of a set of charged bosons in localised states to be the sum of the energies of the bosons in the individual potential wells. The partition function Z for such a system is then the product of the partition functions z for each of the wells, and the system free

energy $F = k_B T \ln Z$ is simply the sum of the individual free energies $k_B T \ln z$. Hence it makes sense to study the partition function for one localised state of energy E on its own. The free energy of all localised bosons is then given by

$$F = k_B T \int_{-\infty}^{0} dE N_L(E) ln z(E), \qquad (5)$$

where $N_L(E)$ is the one-particle density of localised states below the mobility edge.

There is an important reference case when the temperature dependence of the specific heat can be readily established; this occurs when $\nu = 1$ and $\mu = 0$. In that case the repulsive Coulomb energy scales as E, Eq.(4). By introducing $E/k_B T$ as a new variable in the integral, Eq.(5), and assuming that the density of states N_L is energy independent in the region of order T/κ below the mobility edge one obtains

$$C = -T \frac{\partial^2 F}{\partial T^2} \propto T. \qquad (6)$$

In the general case $\nu \neq 1$ and (or) N_L not energy independent the specific heat has a non-linear temperature dependence. In this paper we study the case of low doping when $N_L(\epsilon) = n_L \delta(E - \epsilon)$ where n_L is the number of impurity wells with only one localised level in each of them.

III. CHARGED BOSONS IN A SINGLE LOCALISED STATE

We focus on the properties of a single localised state ϵ. The probability for the state to contain p bosons is proportional to $e^{-\beta(w-p\mu)}$ where μ is the chemical potential and $\beta \equiv 1/k_B T$. (We shall retain the possibility of a non-zero chemical potential until it starts to complicate the equations.) We can re-express $w - p\mu$ as

$$w - p\mu = \kappa (-\epsilon)^\nu (p - p_0)^2 - \kappa (-\epsilon)^\nu p_0^2 \qquad (7)$$

where

$$p_0 = \frac{1}{2} + \frac{\mu - \epsilon}{2\kappa(-\epsilon)^\nu} \qquad (8)$$

Fig 1 shows a graph of $(w-p\mu)/[\kappa(-\epsilon)^\nu]$ as a function of p. The partition function $z(\epsilon)$ for such a single localised state is

$$z(\epsilon) = \sum_{p=0}^{\infty} e^{-\beta(w-p\mu)} \qquad (9)$$

$$= e^{p_0^2 \beta \kappa(-\epsilon)^\nu} \sum_{p=0}^{\infty} e^{-\beta\kappa(-\epsilon)^\nu(p-p_0)^2}. \qquad (10)$$

The partition function is thus completely determined by the dimensionless parameters p_0 and $k_B T/[\kappa(-\epsilon)^\nu]$. The mean occupancy $\langle p \rangle$ is

$$\langle p \rangle = k_B T \frac{\partial \ln z(\epsilon)}{\partial \mu} \qquad (11)$$

and, when $\mu = 0$, the specific heat capacity c is

$$c = \beta^2 \frac{\partial^2 \ln z(\epsilon)}{\partial \beta^2}. \qquad (12)$$

Truncating the series at 100 terms the calculated values of these quantities are shown in Figs 2 and 3. We now attempt to understand these results in more detail, looking separately at each temperature range.

1. $k_B T \ll \kappa (-\epsilon)^\nu$

   At low temperatures the partition function is dominated by the term with p closest to p_0, i.e. the value of p giving the lowest value of $w - p\mu$, and so the mean occupancy $\langle p \rangle$ is an integer and goes up in steps as p_0 increases, as seen in Fig 2a. The changeover in dominance from one term to another occurs when p_0 is a half-integer, at which point the two lowest energy states are degenerate.

   So long as one term dominates the partition function, the specific heat capacity c will be close to zero. However when p_0 is close to a half-integer we have a two level system and a corresponding Schottky anomaly in the specific heat capacity. This is seen in Fig 3a: c is zero when p_0 is equal to a half-integer and rises to a maximum on either side, when the level separation is $\sim k_B T$. Hence, at fixed $k_B T/[\kappa(-\epsilon^\nu)]$, the low temperature specific heat capacity (i.e. $k_B T \ll p_0^2 \kappa(-\epsilon)^\nu$) is periodic in p_0. We also note from Fig. 3 that the peak in the specific heat capacity rises to a maximum when p_0 is an integer. This is because the lowest energy level is the only non-degenerate level, all others being in degenerate pairs; hence, at low temperature, we effectively have a two level system in which the upper level is a degenerate pair, thus resulting in a larger peak in c than occurs in an ordinary two level system.

2. $k_B T > \kappa(-\epsilon)^\nu$

   We can approximate the sum by an integral

   $$z(\epsilon) \approx e^{p_0^2 \beta \kappa(-\epsilon)^\nu} \int_0^\infty dp e^{-\beta\kappa(-\epsilon)^\nu(p-p_0)^2} \qquad (13)$$

   (a) $\kappa(-\epsilon)^\nu < k_B T < p_0^2 \kappa(-\epsilon)^\nu$

   In this case we can approximate the lower limit of the integral as $-\infty$, i.e. the partition function can be approximated by an untruncated gaussian, and is therefore approximately symmetrical about p_0. Hence, in this temperature range we have

   $$\langle p \rangle \approx p_0 \qquad (14)$$

as is clearly seen in Figs 2a and 2b.

After integration, the partition function becomes

$$z(\epsilon) \approx e^{\beta p_0^2(\kappa-\epsilon)^\nu} \sqrt{\frac{\pi k_B T}{\kappa(-\epsilon)^\nu}} \qquad (15)$$

from which we obtain that

$$c \approx \frac{1}{2} k_B \qquad (16)$$

This result is another example of the equipartition theorem of classical statistical mechanics and arises simply because w is proportional to the square of a co-ordinate, namely $p - p_0$. In Fig. 3b the effect of this result is seen in the region around $k_B T \approx \kappa(-\epsilon)^\nu$.

(b) $k_B T > \kappa(-\epsilon)^\nu$ and $k_B T \gg p_0^2 \kappa(-\epsilon)^\nu$

In this case we can make the approximation that

$$\int_0^{p_0} dp\, e^{-\beta \kappa(-\epsilon)^\nu (p-p_0)^2} \approx p_0 \qquad (17)$$

and so the partition function becomes

$$z \approx p_0 + \frac{1}{2}\sqrt{\frac{\pi k_B T}{\kappa(-\epsilon)^\nu}} \qquad (18)$$

As a consequence, the mean occupancy $\langle p \rangle$ becomes proportional to the square root of temperature:

$$\langle p \rangle \approx \sqrt{\frac{k_B T}{\pi \kappa(-\epsilon)^\nu}} \qquad (19)$$

and this gives rise to the increase in $\langle p \rangle$ at large temperatures seen in Fig. 2. Once again, the specific heat capacity $c \approx \frac{1}{2} k_B$, as seen in Fig. 3.

IV. BOSE-GLASS - SUPERFLUID TRANSITION

Here we assume that all the localised states have the same value of ϵ and derive the conditions for the Bose condensate to occur. The most startling conclusion is that, in particular circumstances, it is possible to take a system in which there is no Bose condensate and create one by raising the temperature.

If the de-localised bosons are treated as being free particles of spin-0 and mass m, then at temperature T and when $\mu = 0$, the number of de-localised bosons per unit cell of volume Ω is

$$\left(\frac{T}{T_{c0}}\right)^{\frac{3}{2}}$$

where

$$k_B T_{c0} = 3.3125 \frac{\hbar^2}{m} \left(\frac{1}{\Omega}\right)^{\frac{2}{3}} \qquad (20)$$

If there are n_L localised states in each unit cell and the mean occupancy of each state is $\langle p \rangle$ then the number of localised bosons per unit cell is

$$n_L \langle p \rangle$$

If there are n bosons, in total, per unit cell, then the number of bosons in the Bose condensate is

$$n - n_L \langle p \rangle - \left(\frac{T}{T_{c0}}\right)^{\frac{3}{2}}$$

and the temperature of the phase transition T_c is found by solving

$$n - n_L \langle p \rangle - \left(\frac{T_c}{T_{c0}}\right)^{\frac{3}{2}} = 0. \qquad (21)$$

However, as we have seen, $\langle p \rangle$ is in general a function of T and so solving this equation is not trivial. Nevertheless we can make some simple observations about the conditions necessary for a Bose condensate to occur. Fig. 4 summarises the conclusions.

When p_0 is just above an integer value p_-, $\langle p \rangle$ increases monotonically with temperature (as in Fig. 2b); we then have two possibilities:

1. $n < n_L p_-$

   No Bose condensate occurs at any temperature.

2. $n > n_L p_-$

   In this case equation Eq.(21) has one solution, being the temperature above which the Bose condensate disappears.

When p_0 is just below an integer value p_+, on the other hand, $\langle p \rangle$ no longer increases monotonically with temperature (again, see Fig. 2b); rather, as T increases above zero $\langle p \rangle$ falls from p_+ to p_0 before rising back up again. Now we can distinguish three cases:

1. $n < n_L p_0$

   No Bose condensate occurs at any temperature.

2. $n > n_L p_+$

   At $T = 0$ the Bose condensate is present, but disappears as the temperature is raised.

3. $n_L p_0 < n < n_L p_+$ This is more complicated. At $T = 0$ the Bose condensate is absent. If

$$k_B T_{c0} < \sim \frac{\kappa(-\epsilon)^\nu}{n_L^{\frac{2}{3}}}$$

then the Bose condensate will be absent at all temperatures. If, on the other hand,

$$k_B T_{c0} > \sim \frac{\kappa(-\epsilon)^\nu}{n_L^{\frac{2}{3}}}$$

then a Bose condensate will appear at a temperature $k_B T \sim \kappa(-\epsilon)^\nu$ and disappear as the temperature is raised further.

V. CONCLUSION

We have formulated the statistics of charged bosons partly localised by impurities. A simple form of the partition function is proposed by the use of a reasonable scaling of the Coulomb energy with the localisation length. A non-uniform dependence of the specific heat of the partly localised charged superfluid is found at low temperatures which strongly depends on the exponent ν of the localisation length. The Bose-glass - superfluid transition is analysed (Fig.4) as a function of the n/n_L ratio and the Coulomb interaction as characterised by the parameter p_0. A new phase is found, which is a Bose-glass at $T = 0$ but a superfluid at finite temperatures.

We believe that our findings are relevant for doped high-T_c cuprates having many properties reminiscent of the charged Bose-liquid[1]. Because the level of doping of these Mott-Hubbard insulators is high, one can expect $N_L(E)$ to vary smoothly with energy E (rather than having spikes corresponding to discrete levels). In that case our approach leads to a non-linear temperature dependence of the specific heat at low temperatures if $\nu \neq 1$. From a preliminary analysis, the experimental observation of $C \propto T^{1-\delta}$ in superconducting $La_{2-x}Sr_xCuO_4$[20] appears to be consistent with the existence of bosons partly localised by disorder.

[1] A.S. Alexandrov and N.F. Mott, Rep. Prog. Phys. **57**, 1197 (1994); 'Polarons and Bipolarons' , World Scientific (1995).
[2] M.R. Schafroth, Phys. Rev. **100**, 463 (1955).
[3] L.L.Foldy, Phys.Rev. **124**, 649(1961).
[4] N. Bogoliubov, J.Phys. USSR **11**, 23-32(1947).
[5] R.F.Bishop, J. Low Temp.Phys. **15**, 601(1974).
[6] A.L. Fetter, Ann. Phys. (N.Y.) **64**, 1, (1971).
[7] S.R.Hore and N.E.Frankel, Phys. Rev. B **12**, 2619(1975); ibid **14**, 1952(1976).
[8] D.F.Hines and N.E.Frankel, Phys. Rev. B**20**, 972 (1979).
[9] D.K. Lee and E. Feenberg, Phys. Rev. **137**, A731 (1965).
[10] K.A. Brueckner, Phys. Rev. **156**, 204 (1967).
[11] C-W. Woo and S. Ma, Phys. Rev. **159**, 176 (1967).
[12] A.S. Alexandrov, Phys. Rev. B**48**, 10571 (1993); A.S. Alexandrov *et al*, Phys. Rev. Lett. **76** 983 (1996).
[13] J.A. Hertz, L. Fleishman, and P.W. Anderson, Phys. Rev. Lett. **43**, 942 (1979).
[14] M. Ma, B.I. Halperin, and P.A. Lee, Phys. Rev. B**34**, 3136 (1986).
[15] M.P.A. Fisher, P.B. Weichman, G. Grinstein, and D.S. Fisher, Phys. Rev. B**40**, 546 (1989).
[16] M.P.A. Fisher, G. Grinstein and S.M. Girvin, Phys. Rev. Lett. **64**, 587 (1990).
[17] D.B. Haviland, Y. Liu and A.M. Goldman, Phys. Rev. Lett. **62**, 2180 (1989).
[18] D.K.K. Lee and J.M.F. Gunn, J. Low Temp. Phys. **89**, 101 (1992).
[19] For a review see: M.A. Kastner, Physics Today, **46**, 24 (1993).
[20] N.E. Hussey, J.P. Bird, D.F. Brewer, C.S. McMenamin and A.L. Thomson, Europhys. Lett., **29**, 383 (1995).

FIG. 1. Graph of $(w - p\mu)/[\kappa(-\epsilon)^\nu]$ against p.

FIG. 2. The mean occupancy $\langle p \rangle$ as a function of p_0 and $\log_{10}\{k_B T/[\kappa(-\epsilon)^\nu]\}$. (a) The full 3-D plot. (b) $\langle p \rangle$ versus $\log_{10}\{k_B T/[\kappa(-\epsilon)^\nu]\}$ for selected values of p_0.

FIG. 3. The specific heat capacity c as a function of p_0 and $\log_{10}\{k_B T/[\kappa(-\epsilon)^\nu]\}$. (a) The full 3-D plot. (b) c versus $\log_{10}\{k_B T/[\kappa(-\epsilon)^\nu]\}$ for selected values of p_0: 3.0, 3.2, 3.3, 3.4, 3.48 and 3.5. At low temperatures, c is approximately invariant under $p_0 \to p_0 \pm 1$ and under $p_0 \to n - p_0$ where n is any integer greater than p_0.

FIG. 4. Dependence of the possibility for Bose condensate formation on n/n_L and p_0. In the shaded regions, no Bose condensate can exist at $T = 0$ but as the temperature is raised a condensate may form depending on the value of $n_L^{\frac{2}{3}} k_B T_{c0}/[\kappa(-\epsilon)^\nu]$.